## CONDENSED MATTER, MATERIALS SCIENCE, and CHEMISTRY

## An Implicit Algorithm for a Rate-Dependent Brittle Damage Model

Q. Ken Zuo, T-3

n another paper in this volume [1], we presented a rate-dependent continuum damage model for brittle materials under dynamic loading. In this paper, we will discuss the numerical algorithm for the model. In an analysis code, the total strain rate  $\dot{\epsilon}$  is obtained from the momentum equation and one needs to find the stress rate  $\dot{\sigma}$ . For the current model, the evolution equations for the stress and average crack size (damage) can be written as [1]

$$\dot{\sigma} = \left(\mathbf{C}_m + \mathbf{D}(\overline{c})\right)^{-1} \left(\dot{\varepsilon} - 3\left(\dot{\overline{c}} / \overline{c}\right) \mathbf{D}(\overline{c}) \sigma\right), \quad \text{(1a)}$$

$$\dot{\overline{c}} = \dot{c}_{\text{max}} \left(1 - \frac{1}{1 + \left\langle F(\sigma, \overline{c}) \right\rangle}\right), \quad \text{(1b)}$$

where  $C_m$  is the compliance (4<sup>th</sup>-order tensor) of the matrix (undamaged) material,  $\mathbf{D}(\bar{c})$  is the damage tensor given below;  $\bar{c} = \bar{c}(t)$  is the average crack radius, which evolves with the time. The terminal speed  $\dot{c}_{max}$  for crack growth is either the shear wave speed of the matrix for closed cracks, or the Rayleigh wave speed for open cracks. The angled bracket in Eq. (1b) is the Macaulay bracket, which takes the value of the argument when positive and is zero otherwise. Crack growth ( $\dot{\bar{c}} > 0$ ) occurs when the stress state is outside the damage surface (i.e.,  $F(\sigma,c) > 0$ ). The expression of the damage surface is given in [1].

For an isotropic, linear elastic matrix material, the compliance tensor is  $C_m = 1/(3K)\mathbf{P}^{sp} + 1/(2G)\mathbf{P}^d$ , where K and G are the bulk and shear moduli;  $\mathbf{P}^{sp}$  and  $\mathbf{P}^d$  denote the spherical and deviatoric projection operators, respectively [1]. The damage tensor is related to the average crack radius  $(\bar{c})$  by  $\mathbf{D}(\bar{c}) = \beta^e N_0 \bar{c}^3 \mathbf{P}(\sigma)$  where  $\beta^e = 64\pi(1-\nu)/(15G)$  is a material constant depending on the elastic properties of the undamaged material

( $\nu$  is the Poisson's ratio);  $N_0$  is the crack number density (number of cracks per unit material volume) and  $N_0\bar{c}^3$  is a scalar measure of damage.  $\mathbf{P}(\sigma)$  is a  $4^{\text{th}}$ -order, dimensionless tensor determined by the signs and directions of the principal stresses [2]. The damage is isotropic when the principal stresses are all tensile or all compressive. When the principal stresses have mixed signs, however, the current model predicts anisotropic damage with the directions of tensile principal stresses accumulating more damage than other directions.

Consider a time step  $\Delta t = t^{n+1} - t^n$  with the total strain increment given by  $\Delta \varepsilon = \varepsilon \Delta t$ . Suppose the stress and crack size (radius) at the beginning of the time step are given by  $(\sigma^n, c^n)$ . An implicit algorithm will be used for updating the material state ( $\sigma^{n+1}$ ,  $c^{n+1}$ ). An implicit integration algorithm offers the advantage of placing no additional stability constraint on the size of the time step, which could be an issue for the explicit algorithm (as we will see in Fig. 1). The final crack size  $\bar{c}^{n+1}$  is solved with the following procedure. First, define the trial state by assuming the step is elastic, i.e., there is no crack growth during the step,

 $c^{tr}=c^{\bar{n}}:\sigma^{tr}=\sigma^{n}+(\mathbf{C}_{m}+\mathbf{D}(c^{n}))^{-1}\Delta\varepsilon$ . If both the stress state at the beginning of the time step and the trial stress state are inside or on the damage surface, i.e.,  $F(\sigma^{n},\bar{c}^{n})\leq 0$  and  $F(\sigma^{tr},c^{n})\leq 0$ , then the step is indeed purely elastic. In this case, the trial state is the final solution,  $\bar{c}^{n+1}=\bar{c}^{tr}$ ,  $\sigma^{n+1}=\sigma^{tr}$ . Otherwise, the step involves crack growth and a correction to the trial state is needed. Suppose  $F(\sigma^{tr},c^{n})>0$ , that is, the trial state is outside the damage surface. Applying the backward Euler integration scheme to that evolution equation gives the final stress as

 $\boldsymbol{\sigma}^{n+1}(\overline{c}^{n+1}) = \left(\mathbf{I} + 3\left(1 - \frac{\overline{c}^{n}}{\overline{c}^{n+1}}\right)\left(\mathbf{C}_{m} + \mathbf{D}\right)^{-1}\mathbf{D}\right)^{-1}$   $\left(\boldsymbol{\sigma}^{n} + \left(\mathbf{C}_{m} + \mathbf{D}\right)^{-1}\Delta\varepsilon\right)$ (2)

where the relationship  $\dot{c}\Delta t = \bar{c}^{n+1} - c^n > 0$  has been used, and the dependency of  $\mathbf{D}(c^{n+1})$  on  $c^{n+1}$  has been dropped for compactness. With the material state

## **CONDENSED MATTER, MATERIALS SCIENCE, and CHEMISTRY**

at the beginning of the step  $(\sigma^n, c^n)$  and the strain increment  $(\Delta \varepsilon)$  given and fixed, the final stress  $\sigma^{n+1}$  is a function of the final crack size  $c^{n+1}$  only. Applying the central difference scheme (the trapezoidal rule) to the evolution equations for the crack size [Eq. (1b)] yields

 $\frac{\overline{c}^{n+1} - \overline{c}^{n}}{\dot{c}_{\max} \Delta t} - \left(1 - \frac{1}{1 + \frac{1}{2} \left(F(\sigma^{n+1}, \overline{c}^{n+1}) + \left\langle F(\sigma^{n}, \overline{c}^{n}) \right\rangle \right)}\right) = 0.$ (3)

With  $\sigma^{n+1}$  given by Eq. (2) as a function of  $c^{n+1}$  only, Eq. (3) is a nonlinear equation for  $\overline{c}^{n+1}$ , which can be solved by an iterative method, using the trial state ( $\sigma^{tr}$ , $c^n$ ) as the starting state for the iteration.

Figure 1 compares the model predictions using the implicit and explicit algorithms with four different time steps (from 0.01ns to 10 ns). The loading is uniaxial strain with a strain rate of  $\varepsilon_{11} = 10^5/\text{s}$ , and the model material is

silicon carbide ceramic [1]. As the time step is reduced, both the implicit and explicit algorithms converge to the same result (the curve in the middle with  $\Delta t \leq 0.1$ ns). It is also shown that the implicit algorithm gives a more accurate result for large time steps. For  $\Delta t = 10$  ns (corresponding to a strain increment of  $\Delta \epsilon_{11} = 10^{-3}$ ), the explicit algorithm produces severe oscillations.

For more information contact Ken Zuo at zuo@lanl.gov.

[1] Q. Ken Zuo, et al., "A Rate-Dependent Damage Model for Brittle Materials under Dynamic Loading," in this volume on p. 58. [2] Q.H. Zuo, et al., "A Rate-Dependent Damage Model for Brittle Materials Based on the Dominant Crack," *Int. J. Solids Struct.*, in press, pp. 1–31 (2005) (available online at the journal's website.)

**Funding Acknowledgements** NNSA's Advanced Simulation and Computing (ASC) Program.

Fig. 1.
Comparison of the predicted stress-strain responses using implicit (I.) and explicit (E.) algorithms with four time-step sizes:
10 ns, 1 ns, 0.1 ns, and 0.01 ns.



